2-(4-Phenoxyphenyl)propanoic acid

Inchi: InChI=1S/C15H14O3/c1-11(15(16)17)12-7-9-14(10-8-12)18-13-5-3-2-4-6-13/h2-11H,1H3
InchiKey: CQWOKJLMSWMOCJ-UHFFFAOYSA-N
Formula: C15H14O3
SMILES: CC(C(=O)O)c1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 242.27

Physical Properties

Property code	Value	Unit	Source
gf	-82.57	kJ/mol	Joback Method
hf	-293.65	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.667		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	2067.00		NIST Webbook
tb	768.97	K	Joback Method
tc	993.24	K	Joback Method
tf	442.15	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.65	J/mol×K	768.97	Joback Method
cpg	570.72	J/mol×K	955.86	Joback Method
cpg	562.12	J/mol×K	918.48	Joback Method
cpg	552.66	J/mol×K	881.10	Joback Method
cpg	542.29	J/mol×K	843.73	Joback Method
cpg	530.97	J/mol×K	806.35	Joback Method
cpg	578.51	J/mol×K	993.24	Joback Method
dvisc	0.0000251	Pa×s	768.97	Joback Method
dvisc	0.0000368	Pa×s	714.50	Joback Method

dvisc	0.0000575	Pa×s	660.03	Joback Method
dvisc	0.0000973	Pa×s	605.56	Joback Method
dvisc	0.0001828	Pa×s	551.09	Joback Method
dvisc	0.0003944	Pa×s	496.62	Joback Method
dvisc	0.0010286	Pa×s	442.15	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31686&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume